

Development of Finely Discretized Lattice Models for Real Fluids

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The focus of this paper is on development of finely discretized lattice models for simulations of technologically important properties of fluids and their mixtures. Of particular interest are phase coexistence properties, critical parameters (critical temperature, critical density and critical pressure) and second virial coefficients. Monte Carlo simulations in the grand canonical ensemble combined with histogram reweighting techniques are used for the calculations. Critical parameters are determined from mixed finite-size scaling methods. It has been previously demonstrated that finely discretized lattice models have essentially identical thermodynamic and structural properties to their continuum counterparts within simulation uncertainties for some model polar and non-polar fluids [1,2]. The models utilize the Buckingham exponential-6 potential to describe nonbonded non-polar interactions while Coulombic forces treated with Ewald summation are used for polar interactions. We are now interested in numerical equivalence of lattice and continuous space models for polar fluids such as ammonia, carbon dioxide and water. We also study the solvation of ionic solutes in a polar solvent such as water. The hydration of different ion pairs such as NaCl in water at different dilutions close to the critical condition is being investigated in detail. The solvation shell structure and mean ionic activity coefficients are among the properties of interest for the solute-solvent polar mixtures.

[1] A. Z. Panagiotopoulos and S. K. Kumar, Phys. Rev. Lett. 83, 2981 (1999).

[2] A. Z. Panagiotopoulos, J. Chem. Phys. 112, 7132 (2000).